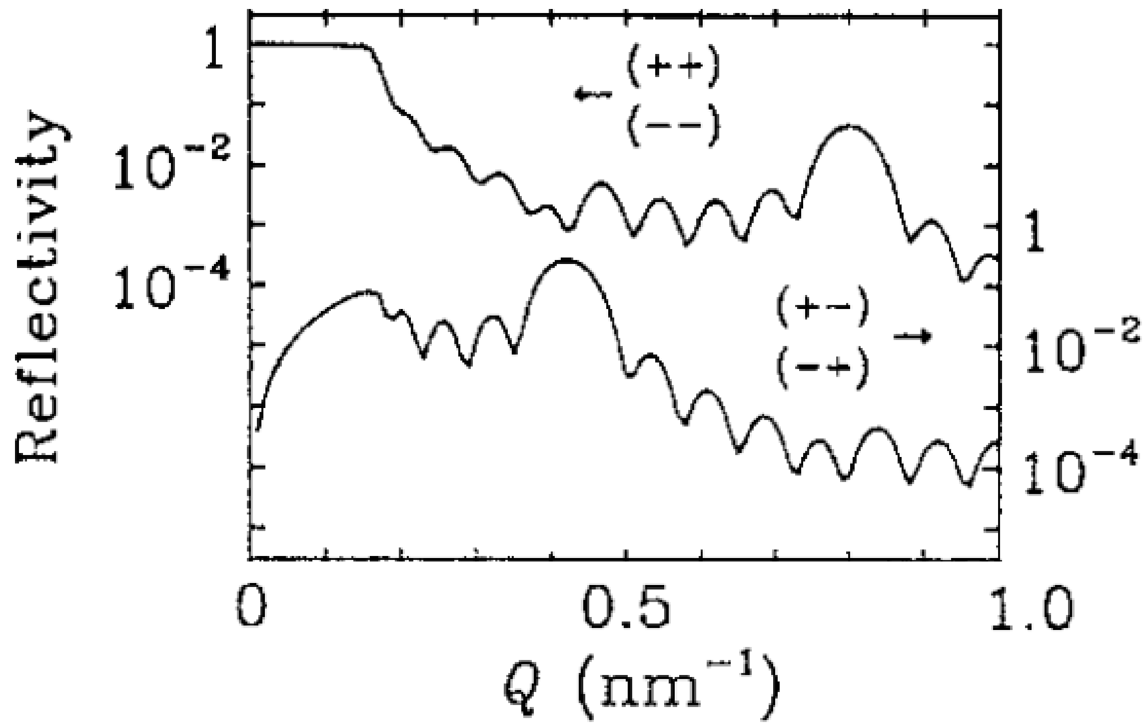

Magnetic Neutron Reflectometry

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9/14/11

Outline

- Scattering processes
- Reflectivity of a slab of material
- Magnetic scattering
- Off-specular scattering
- Source parameters
- Comparison with x-rays

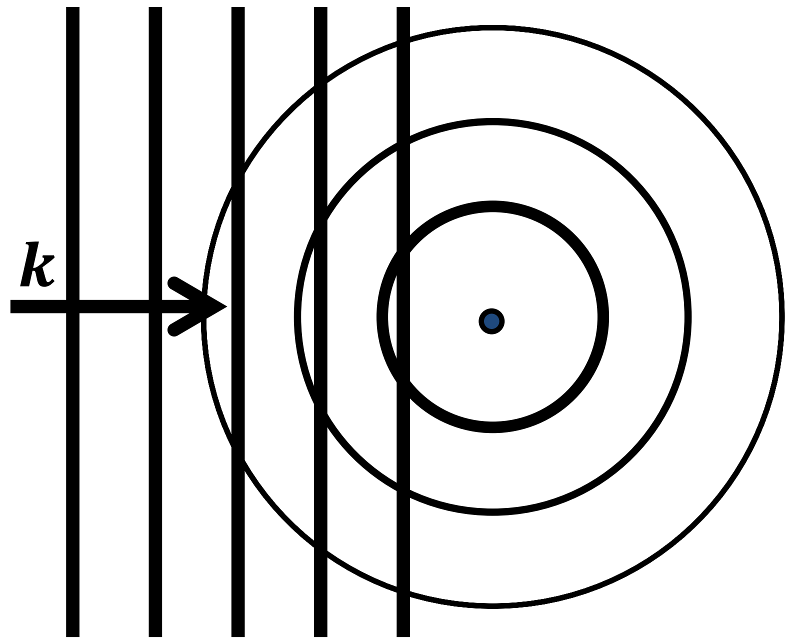
Neutrons are waves

- de Broglie wavelength: $\lambda = \frac{h}{p} = \frac{h}{mv}$
  - Example: $\lambda = 2\text{Å}\,,\ v = 1978\frac{m}{s}\ ,$

$$E = \frac{mv^2}{2} = 20.5\,meV$$

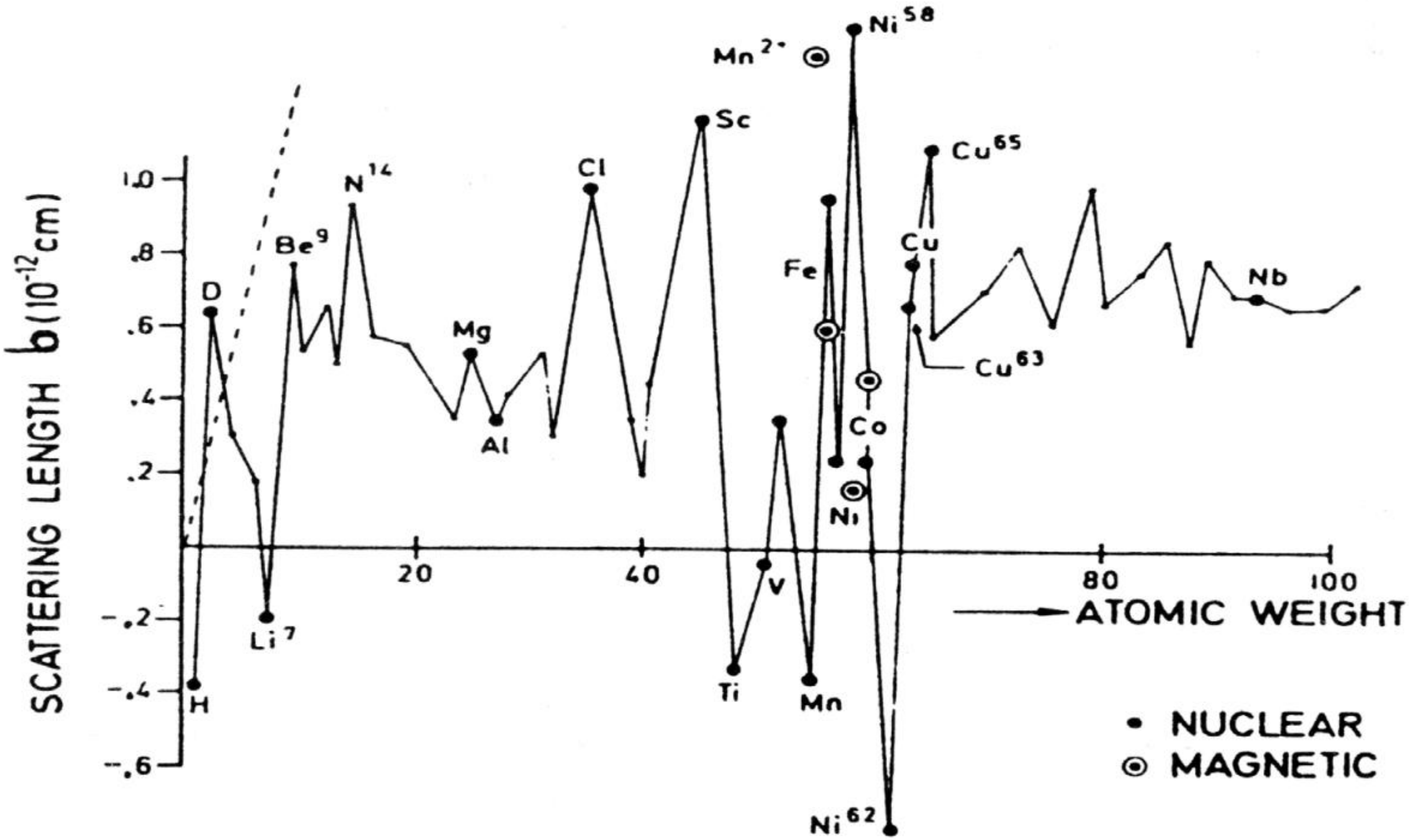
- Plane wave: $\psi \sim e^{i\boldsymbol{k}\cdot\boldsymbol{r}},\ k = \frac{2\pi}{\lambda}$

Scattering from a single fixed nucleus



- Incident plane wave: $\psi \sim e^{ikx}$
- Potential from nucleus: $V(\boldsymbol{r}) = \frac{2\pi\hbar^2}{m} b\ \delta(\boldsymbol{r})$
- Outgoing spherical wave $\psi \sim -\frac{b}{r} e^{ikr}$
- Differential cross section: $\frac{d\sigma}{d\Omega} = b^2$, $b =$ scattering length

Intrinsic Cross Section: Neutrons



Source: Sinha lecture

Reflectometry: Neutrons in media

- Neutrons incident on a slab of material at grazing angle
- Average scattering length density:

$$\rho = \sum_i \; N_i \, b_i$$

  - Neutrons sample average in-plane density

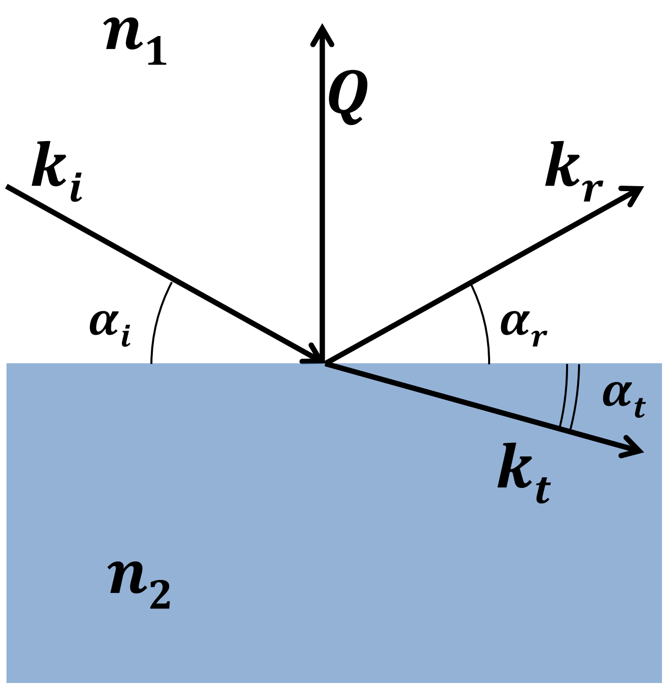
$$\rho(z) = \langle \rho(x, y, z) \rangle_{xy}$$

- Elastic scattering
  - Energy in vacuum: $E = \frac{\hbar^2 {k_0}^2}{2m}$
  - Energy in medium: $E = \frac{\hbar^2 k^2}{2m} + V = \frac{\hbar^2}{2m}(k^2 - 4\pi\rho)$
- Index of refraction:

$$n = \frac{k}{k_0} = 1 - \frac{4\pi}{{k_0}^2}\rho = 1 - \frac{{\lambda_0}^2}{2\pi}\rho$$

- ρ is typically on the order of 10^{-6}Å^{-2}

Fresnel Reflectivity



- Specular reflection:

$$\alpha_r = \alpha_i$$

$$\boldsymbol{Q} = 2k_{iz}\hat{z} = \frac{4\pi}{\lambda}\sin(\alpha_i)\hat{z}$$

- Reflection coefficient: ratio of reflected amplitude to incident amplitude

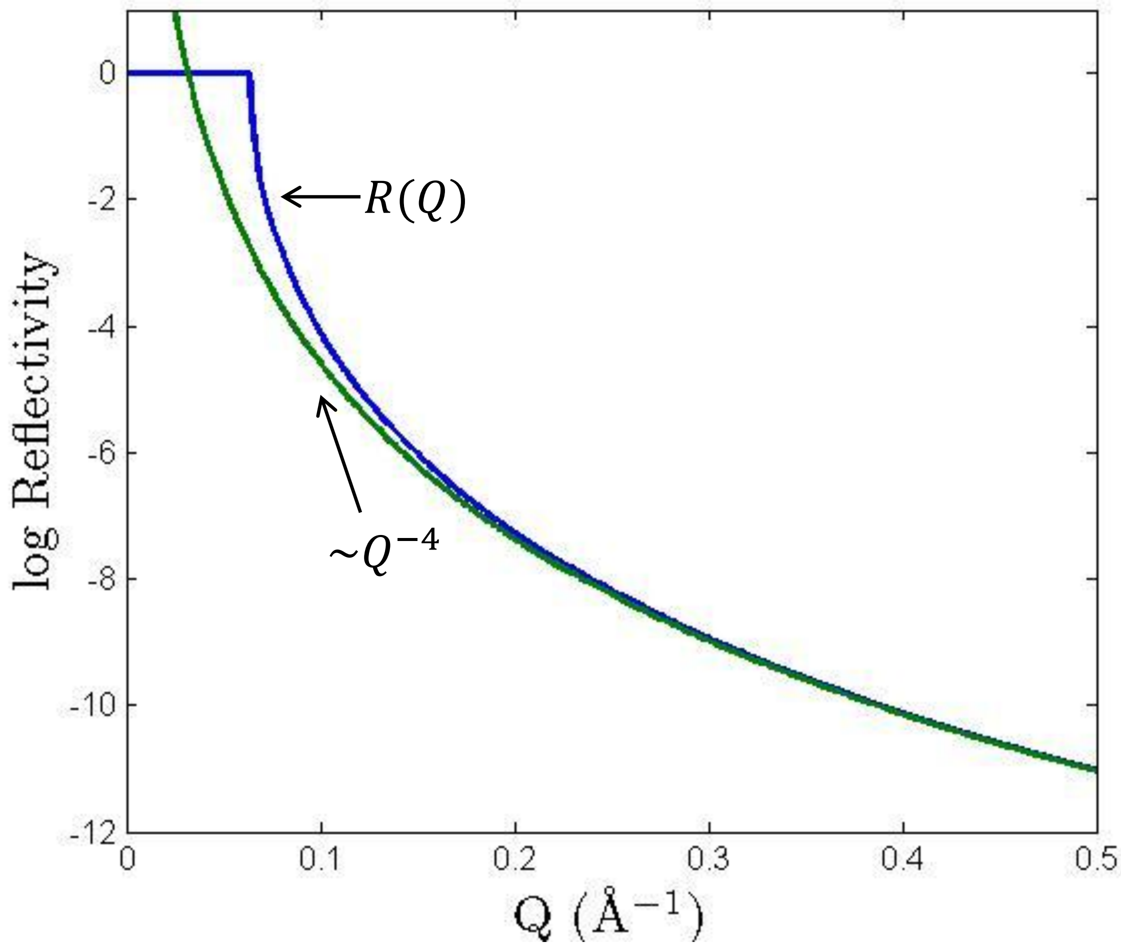
$$r = \frac{k_{iz}-k_{tz}}{k_{iz}+k_{tz}} = \frac{1-\sqrt{1-\left(\frac{Q_c}{Q}\right)^2}}{1+\sqrt{1-\left(\frac{Q_c}{Q}\right)^2}}$$

- Reflectivity:

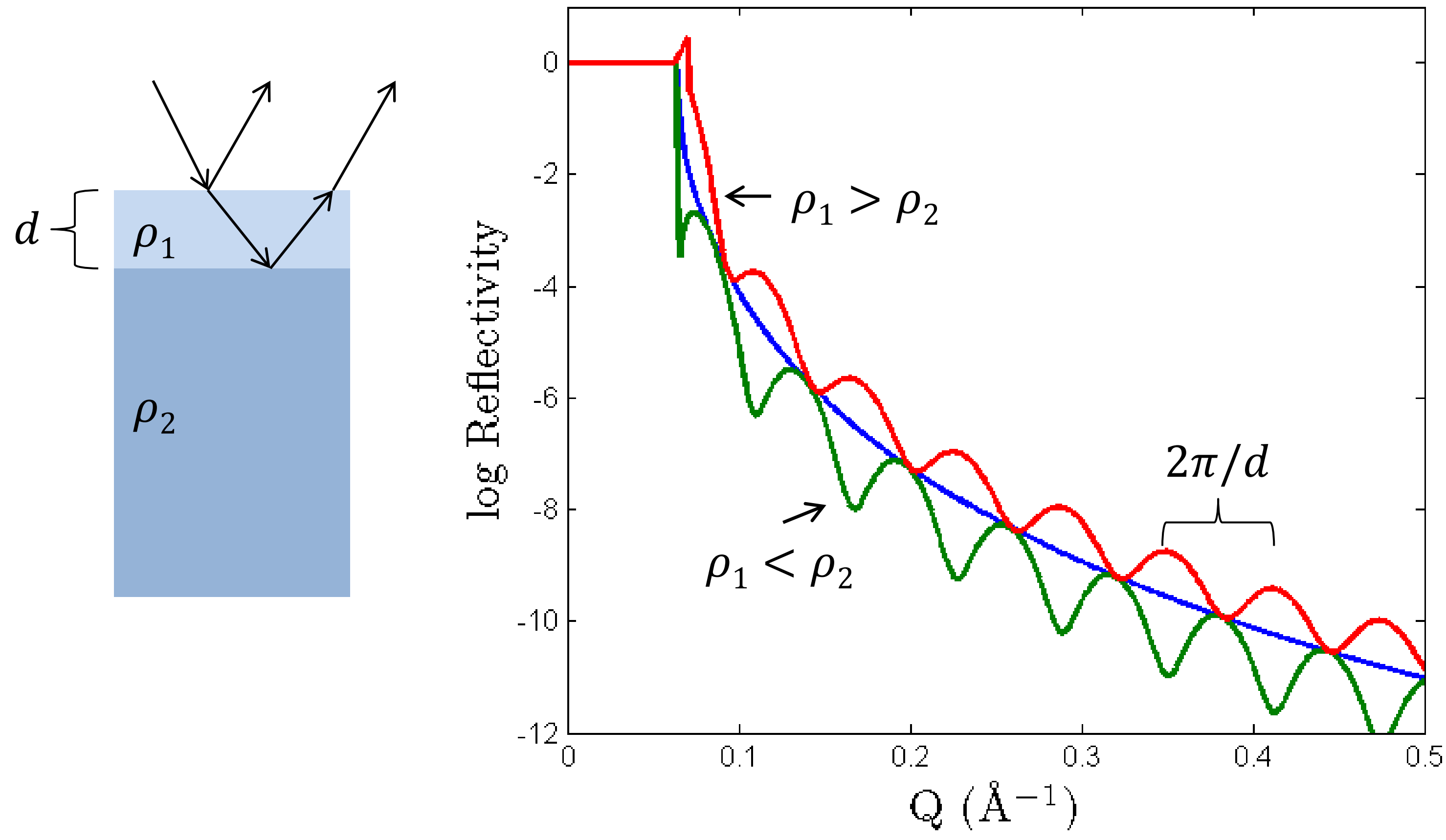
$$R = |r|^2 \approx \left(\frac{Q_c}{2Q}\right)^4 \; for\; Q \gg Q_c$$

$$Q_c{}^2 = 16\pi\rho$$

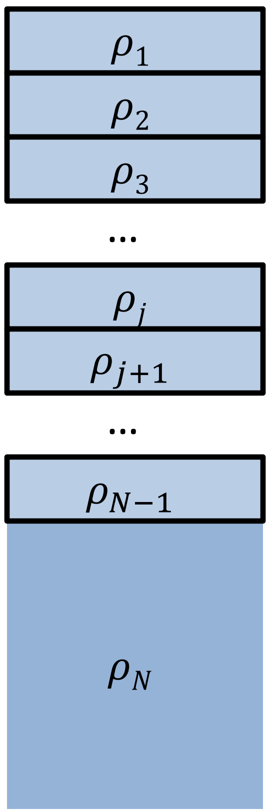
Fresnel Reflectivity



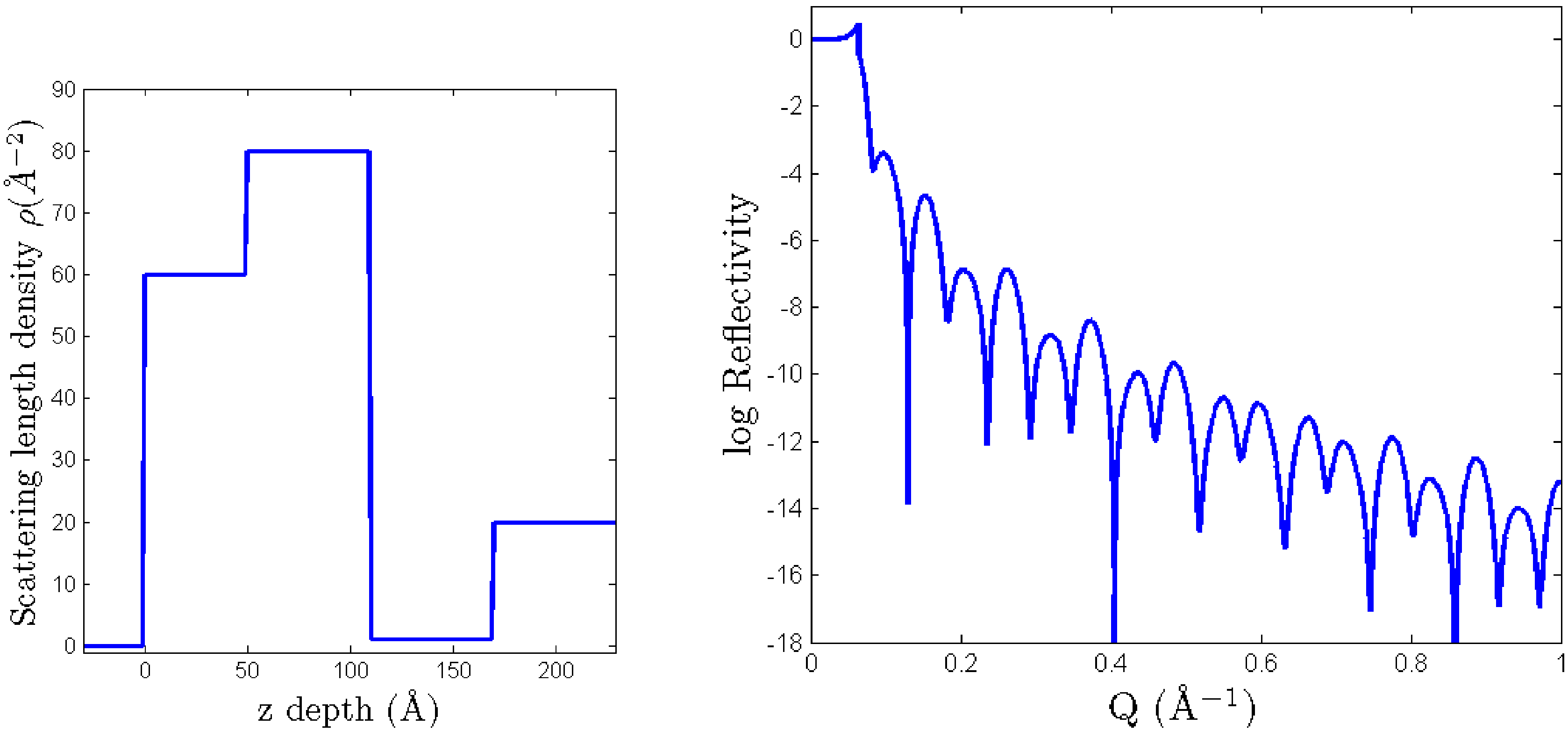
Thin film on a substrate: Kiessig fringes



Multilayer: Parratt formula



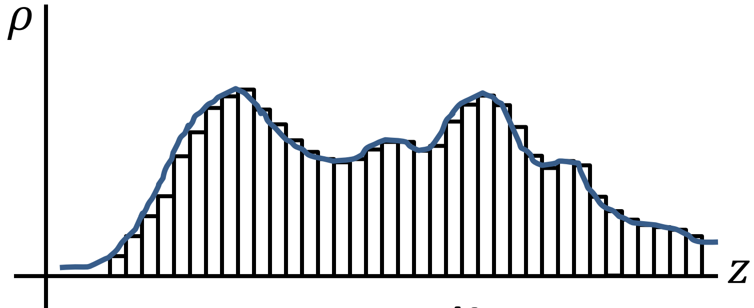
- Net reflectivity at the surface can be calculated *exactly* by enforcing continuity at each interface
- Dynamical: accounts for transmission and reflection at each interface



Scattering length density $\rho(\text{Å}^{-2})$
z depth (Å)
log Reflectivity
Q (Å^{-1})

Reflectivity from an arbitrary $\rho(z)$

- Divide up $\rho(z)$ into slices of constant ρ and apply Parratt formula
  - e.g.



- Or: apply Born approx. (kinematical treatment)

$$r(Q) \approx \frac{4\pi}{iQ} \int_{-\infty}^{\infty} \rho(z) e^{iQz} dz$$

  - Assumes scattering is weak. Fails near Q_c where reflectivity approaches unity (strong scattering)

Inverting Reflectivity Data

- How do you get $\rho(z)$ from $R(Q)$?
  - Start with a good model and refine parameters
  - Inverse Fourier transform: phase can be recovered by adding reference layers of known density to the front & back of the film (Majkrzak 1995)

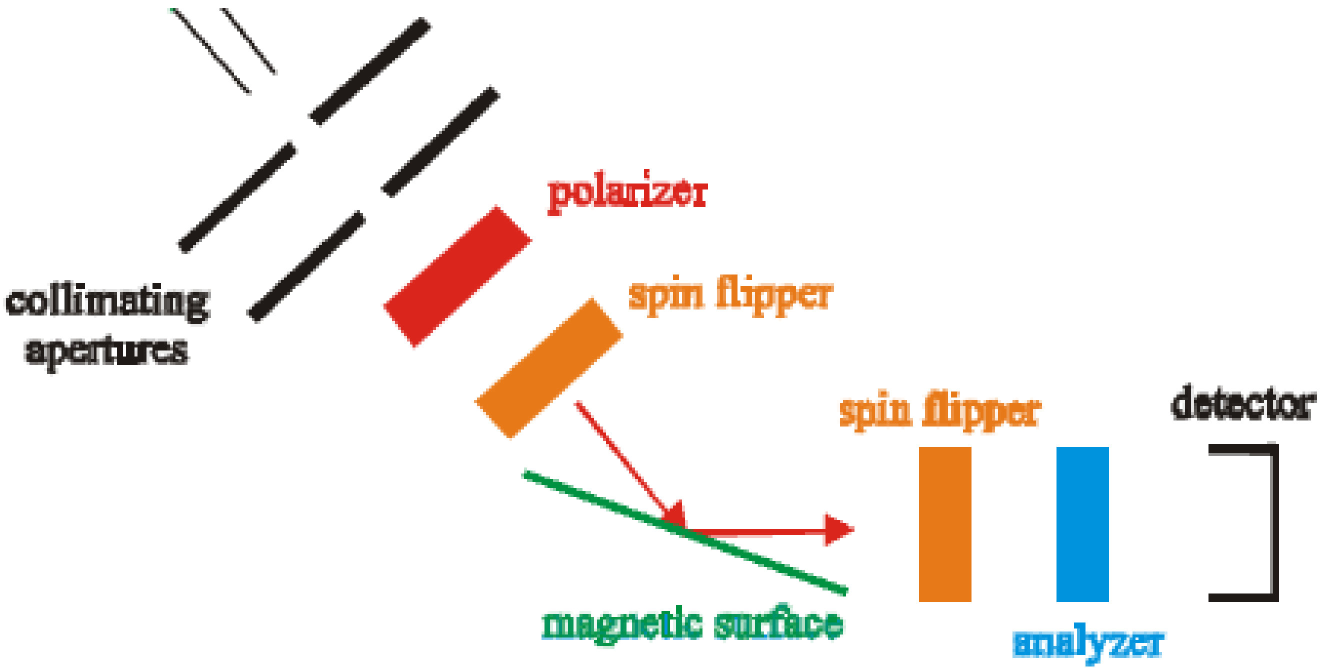
Magnetic reflectometry

- A magnetic field adds a spin-dependent potential to the Schrödinger equation

$$V_m = -\boldsymbol{\mu} \cdot \boldsymbol{B} = -\mu\boldsymbol{\sigma} \cdot \boldsymbol{B}$$

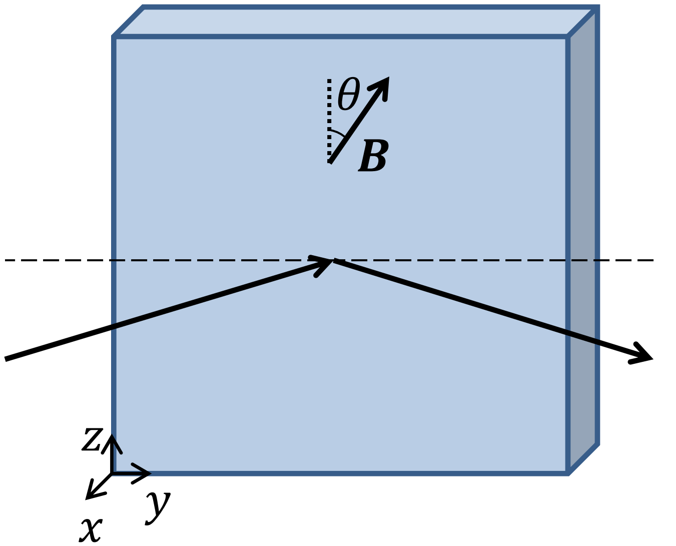
  - μ is the neutron magnetic moment
  - $\boldsymbol{\sigma}$ has the Pauli spin matrices as components
- We now have to treat the incoming plane wave as a spinor: $\psi = \binom{\psi_+}{\psi_-}$
  - Polarizers and analyzers allow control of which spin hits the sample as well as which spin is detected

SNS BL4a Schematic



Magnetic reflectometry

- Let z be the spin quantization axis, and let x lie along $\boldsymbol{Q}$
- Only the components of $\boldsymbol{B}$ perpendicular to $\boldsymbol{Q}$ contribute to scattering



- This gives rise to a set of coupled Schrödinger equations for ψ_+ and ψ_-

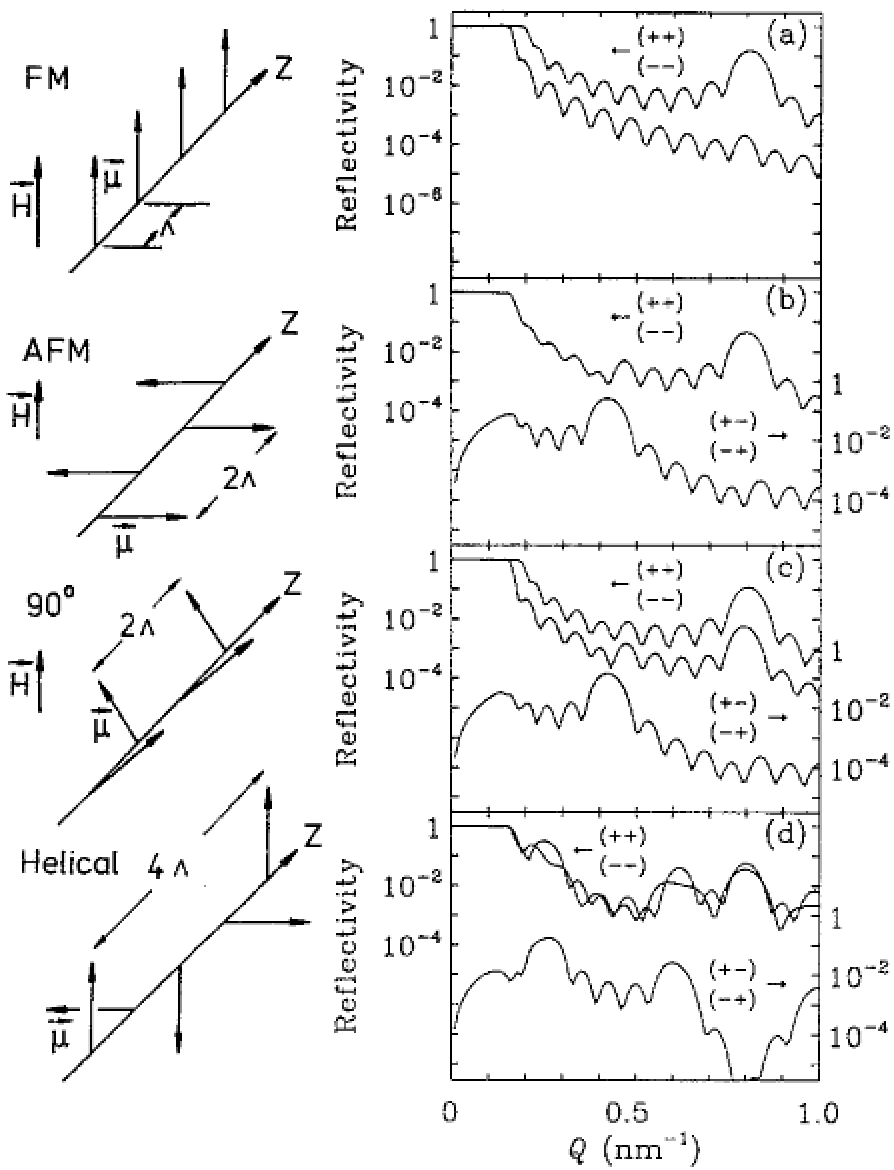
$$[\partial_x{}^2 + k_{0x}{}^2 - 4\pi\rho_{++}]\psi_+ - 4\pi\rho_{+-}\psi_- = 0$$
$$[\partial_x{}^2 + k_{0x}{}^2 - 4\pi\rho_{--}]\psi_- - 4\pi\rho_{-+}\psi_+ = 0$$

$$\rho_{\pm\pm} = \rho_n \pm \frac{m}{2\pi\hbar^2}\mu B_z\,; \quad \rho_{\pm\mp} = \frac{m}{2\pi\hbar^2}\mu(B_x \mp iB_y)$$

Magnetic reflectometry

- ρ_{+-} and ρ_{-+} cause spin flips during scattering
- If $\boldsymbol{B}$ is parallel to $\hat{z}$, then the equations decouple and there is no spin flipping. Then we can treat each polarization separately.
- For arbitrary $\boldsymbol{B}(z)$ we can solve for the reflectivity numerically using an approach similar to the Parratt formalism (Felcher 1987)
- Corrections must be applied for incomplete beam polarization

Magnetic reflectometry



- Simulations: alternating Fe/Cr layers, each 4nm thick. 20 layers total.
- Magnetism only in Fe layers

Zabel 1994

Non-specular reflection

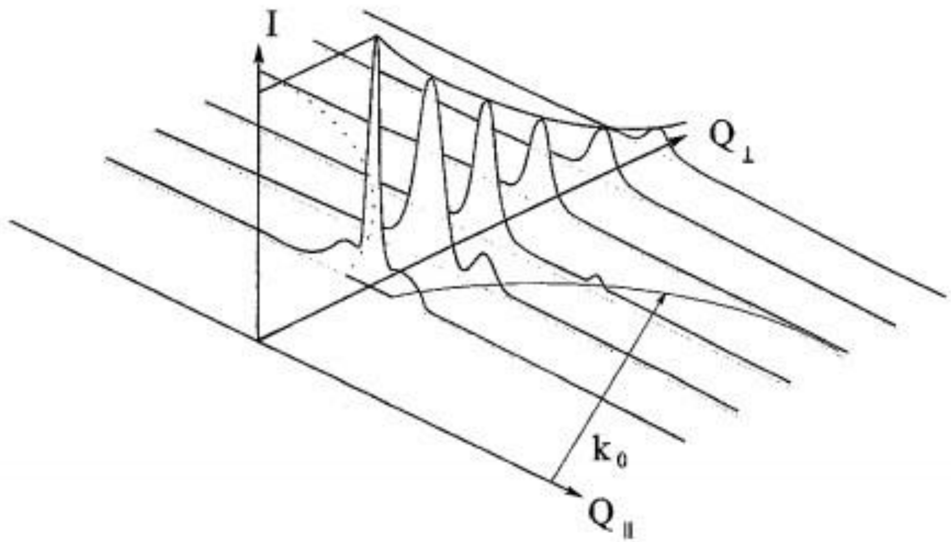


Fig. 7. Schematic view of the specular and off-specular intensity in the reciprocal space parallel to the scattering plane and for a single rough surface. In scans parallel to $Q_\perp$ the specular intensity is probed, in the directions parallel to $Q_\parallel$ the diffuse intensity from the in-plane roughness is examined. The *circles* indicate the location where the transmission coefficients $|t(\phi)|^2$ have maxima, causing the diffuse scattering to exhibit peaks, so called angle's wings or Yoneda peaks

Zabel 1994

- Diffuse scattering from interfacial roughness (Sinha 1988)
- Off specular peaks from in-plane order
  - Also Yoneda peaks near the critical angle, where the transmission coefficient is maximized
- Sensitive to components of $\boldsymbol{B}$ normal to plane

What about x-rays?

- Brighter, more coherent sources
- Element specificity
- Unaffected by external magnetic fields
- Lower penetration depth
- Insensitive to light elements
- Magnetic scattering much weaker than charge scattering

Spallation Neutron Source (ORNL)

- Proton accelerated into mercury target, neutrons knocked loose
- Neutrons come out in pulses (60 Hz)
- Moderator gives them a thermal distribution of velocities
- Detector uses time of flight methods to determine Q

SNS BL4a Fact Sheet

- Wavelength range: $1.8\text{Å} < \lambda < 14.0\text{Å}$
- Q range: $0 < Q < 0.4\text{Å}^{-1}$
- Minimum reflectivity: 10^{-8}
- Magnetic field max
  - $1.2\ T$ with a gap of $50\ mm$
  - $3\ T$ with a gap of $10\ mm$
- Temperature range: $5 – 750\ K$

References

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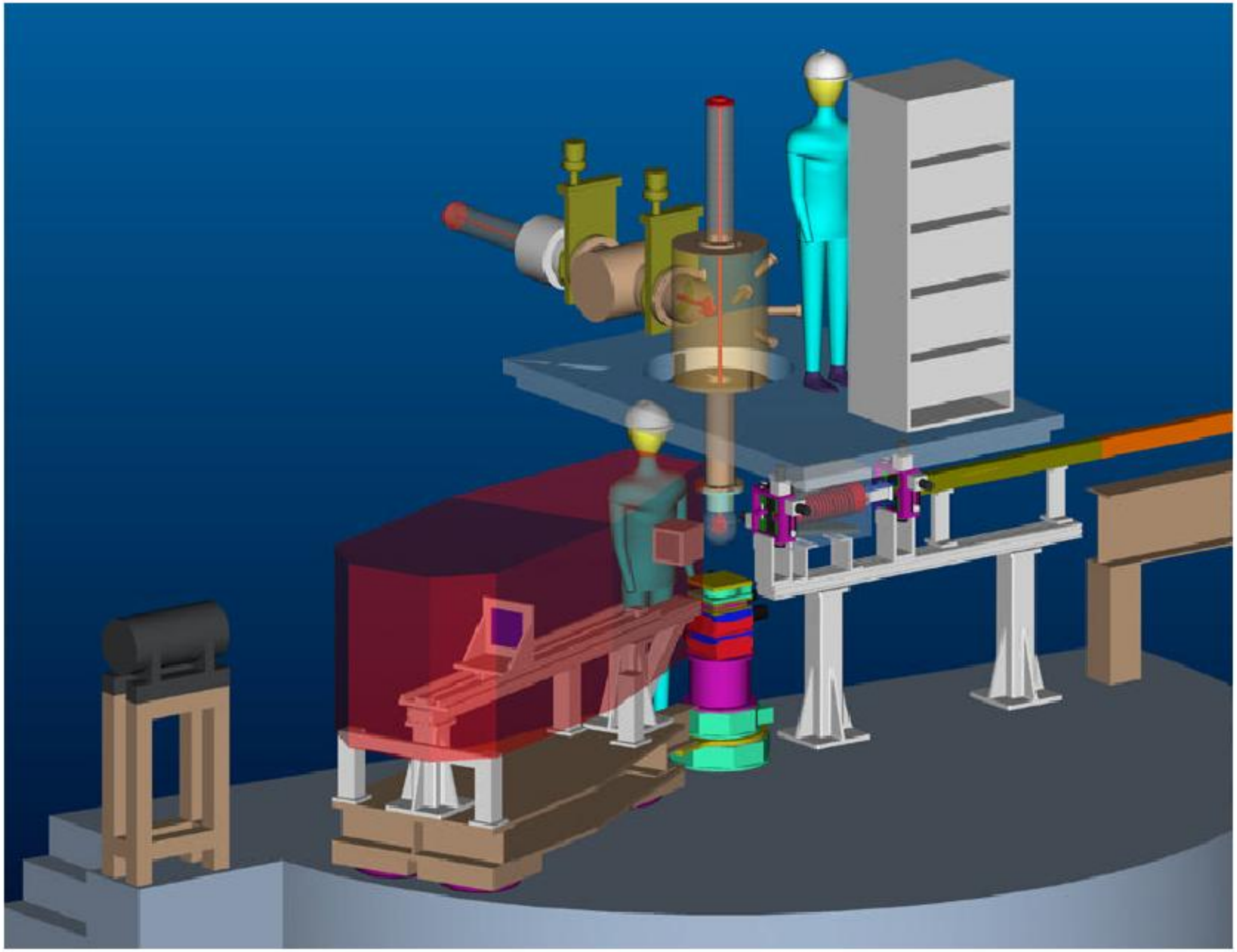
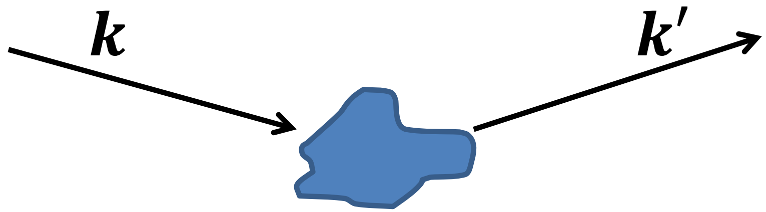
- Lectures by Majkrzak, Sinha, Pynn



UHV system for in-situ polarized reflectometry experiments on ultrathin magnetic films (for clarity reasons the sample magnet is suppressed).

Scattering from many nuclei



- $\boldsymbol{q} = \boldsymbol{k}' - \boldsymbol{k}$
- $\frac{d\sigma}{d\Omega} = \sum_{ij} b_i b_j e^{\iota \boldsymbol{q}\cdot(\boldsymbol{r}_i - \boldsymbol{r}_j)}$
- Ensemble average: $\frac{d\sigma}{d\Omega} = \langle b \rangle^2 S(\boldsymbol{q})$
- $S(\boldsymbol{q}) = \left\langle \sum_{ij} e^{\iota \boldsymbol{q}\cdot(\boldsymbol{r}_i - \boldsymbol{r}_j)} \right\rangle = \langle \hat{\rho}_n(\boldsymbol{q}) \hat{\rho}_n{}^*(\boldsymbol{q}) \rangle$
- $\hat{\rho}_n(\boldsymbol{q})$ is the Fourier transform of nuclear density